#### **Modeling Lean Premixed Combustion in Gas Turbines**

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#### Abstract

A new model has been developed for simulating steady-state, turbulent, gaseous combustion in practical, three-dimensional devices. Although the model was specifically developed for lean, premixed combustion of natural gas in gas turbines, it has general applicability to a variety of gaseous combustion problems and configurations. The model uses a hybrid Eulerian/Lagrangian approach with the Monte Carlo velocity-scalar pdf method coupled to an unstructured-grid flow solver. It was developed from the foundation of PCGC-3, a three-dimensional gas and particle combustion code (Hill and Smoot, 1993), and PDF2DS, a two-dimensional velocity-scalar pdf code (Correa and Pope, 1992). The flow solver calculates the flowfield for an assumed density field and the Monte Carlo pdf solver solves the transport equation for the joint pdf of velocity and scalars.

The unstructured-grid flow solver uses primitive variables (u, v, w, p). It solves the incompressible, Navier-Stokes equations using a co-located, equal-order, control volume-based, finite-element method (Prakash and Patankar, 1985). The mass-weighted, skewed, upwind scheme of Schneider and Raw (1986) is used for the advection terms, while linear interpolation functions are used for the diffusion, pressure gradient and source terms. Rotational periodic boundary conditions are included. The discretized algebraic equations are solved using an iterative, tri-diagonal matrix algorithm. Turbulence is modeled using the k-model. Convective and radiative heat losses are modeled using a wall function method and a discrete ordinates radiation model (Jamaluddin and Smith, 1988), respectively. Turbulence/chemistry interactions are modeled using the velocity-composition, Monte-Carlo pdf approach (Pope, 1985). The pdf calculation includes a new chemical mechanism that was developed specifically for the conditions of lean premixed combustion of natural gas in land-based turbines (Mallampalli, et al., 1996).

In support of the modeling effort, an experimental program has been conducted to collect *in situ* data in a swirling, turbulent, premixed natural gas flame in an atmospheric pressure, laboratory-scale gas turbine combustor (LSGTC). These measurements have included multiple, instantaneous, CARS measurements of gas temperature and major species concentrations (CO, CO<sub>2</sub>, O<sub>2</sub>, and N<sub>2</sub>); multiple instantaneous LDA measurements of axial, tangential, and radial velocity; and multiple instantaneous PLIF images of selected combustion intermediates (OH, and CH). Results are in the form of mean and standard deviation isocontour maps of gas temperature, selected species concentration, and mean and instantaneous PLIF images of OH and CH. These data are being collected at medium and high swirl numbers (SN = 0.74 and 1.29) and at fuel equivalence ratios of 0.65 and 0.80. The poster paper presents example results for the fuel-lean case (= 0.65) at the high swirl number (SN = 1.29).

The velocity-composition pdf model, coupled with a mean flow CFD model, was used to describe the turbulent fluid flow, heat transfer, chemistry, and their interactions in the swirling, lean premixed, methane-

air combustor described above. A premixed natural gas flame was stabilized in the axi-symmetric, laboratory-scale, gas-turbine combustor (LSGTC). A reduced, 5-step chemical mechanism, for describing fuel oxidation and NO chemistry, was used in this LSGTC model. NO emissions from thermal, N2Ointermediate, and prompt pathways were described in this 5-step mechanism. The chemistry calculations were performed efficiently with an in-situ look-up table. An axi-symmetric, unstructured grid, consisting of 2283 vertices and 4302 triangular elements, was used for solving the Eulerian, mean flow equations and the vertices were used to store mean statistics for solving the Lagrangian, fluid particle ( 310,000 fluid particles) equations. Predicted velocity and composition statistics were compared to measurements in the LSGTC for lean equivalence ratios of 0.8 and 0.65. The comparisons of predicted mean velocity and temperature were reasonably good throughout the combustor. The location and magnitude of peak axial velocity was well represented by the model at near inlet regions, though the negative mean axial velocity in the internal recirculation zone was over-predicted. The predicted maximum mean temperature and the penetration zone of the cold, unburned fluid were in reasonable agreement with the experimental data. Correct trends in CO and NO with equivalence ratio were predicted with the model. The *in situ* tabulation method was used to represent the chemical kinetics in this axi-symmetric combustor without requiring significant CPU time and memory.

The model has also been evaluated with premixed combustion data from laboratory flames stabilized by swirl, bluff-body, and a pilot flame (Cannon et al., 1997), and it has been applied to several practical, industrial, gas turbine premixers and combustors (Meng et al., 1997).

#### References

Cannon, S.M., Brewster, B. S., and Smoot, L. D., "Stochastic Modeling of CO and NO in Premixed Methane Combustion," Accepted for Publication in *Combustion and Flame* (1997)

Correa, S. M., and Pope, , S. B., "Comparison of a Monte Carlo/Finite Volume Mean Flow Model with Bluff-Body Raman Data," *Twenty-Fourth Symposium (International) on Combustion/The Combustion Institute*, Pittsburgh, PA, pp. 279-285 (1992)

Hill, S. C., and Smoot, L. D., "A Comprehensive Three-Dimensional Model for Simulation of Combustion Systems: PCGC-3," *Energy and Fuels*, **7**, 874-883 (1993)

Jamaluddin, A S., and Smith, P. J., "Discrete-Ordinates Solution of Radiative Transfer Equation in Non-Axisymmetric Cylindrical enclosures," Proceedings of the 1988 National Heat Transfer Conference, ASME, **96**, 227-232 (1988)

Mallampalli, H. P., Fletcher, T. H., and Chen, J. Y., "Evaluation of CH<sub>4</sub>/NO<sub>X</sub> Global Mechanisms Used for Modeling Lean Premixed Turbulent Combustion of Natural Gas," Western States Section of the Combustion Institute, (96F-098), Livermore, CA (1996)

Meng, F. L., Brewster, B. S., and Smoot, L. D., "Comprehensive Model for Lean Premixed Combustion in Industrial Gas Turbines-Part II - Application," Western States Section of the Combustion Institute, (97S-041, Livermore, CA (1997)

Pope, S. B., "PDF Methods for Turbulent Reactive flows," *Progress in Energy and Combustion Science*, **11**, 119-192 (1985)

Prakash, C., and Patankar, S. V., "A Control Volume-Based Finite-Element Method for Solving the Navier-Stokes Equations Using Equal-Order Velocity-Pressure Interpolation," *Numerical Heat Transfer*, **8**, 259-280 (1985)

Schneider, G. E., and Raw, M. J., "A Skewed, Positive Influence Coefficient Upwinding Procedure for Control-Volume-Based Finite-Element Convection-Diffusion Computation," *Numerical Heat Transfer*, **9**, 1-26 (1986)

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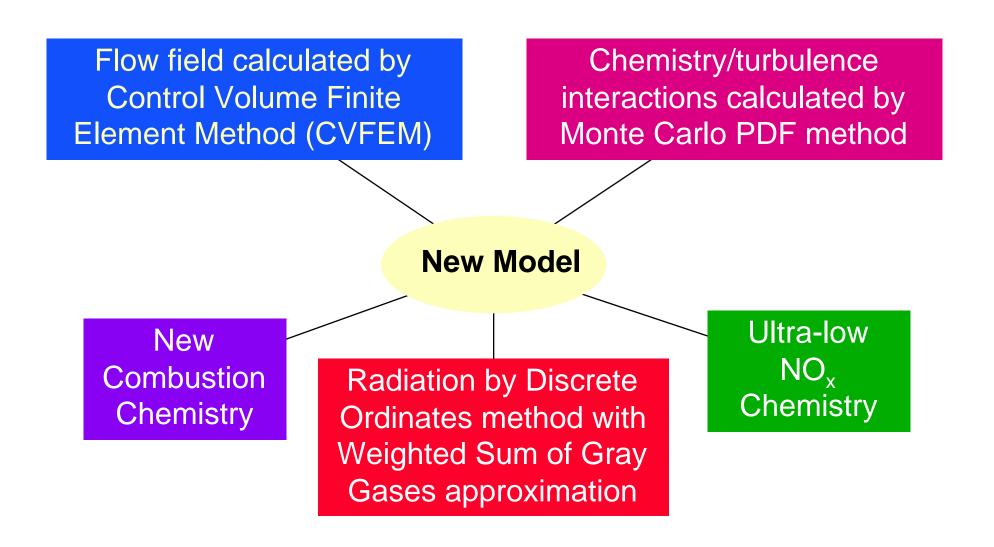
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### **Objectives**

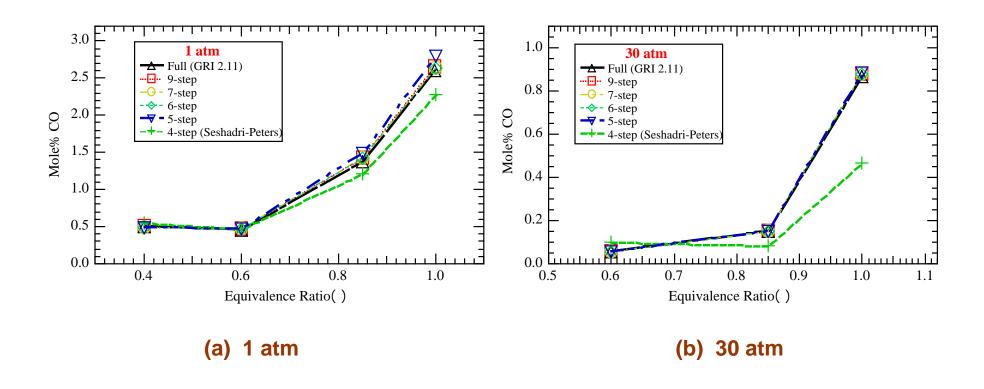
- Develop an improved model for advanced gas turbine systems
  - 3-dimensional
  - Curved boundaries
  - Submodel development for lean premixed systems
- Obtain data for model evaluation
- Evaluate the model
- Apply the model to practical systems
- Provide training and distribute the code

### **Critical Elements of the New Model**



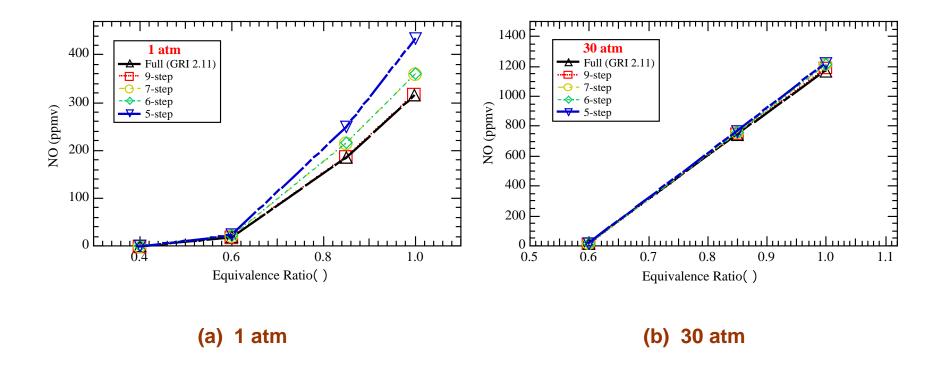
# PSR Predictions of CO at 1 and 30 atm

 $T_{inlet} = 600 \text{ K}, \text{ and } = 2 \text{ ms}$ 



# PSR Predictions of NO at 1 and 30 atm

 $T_{inlet} = 600 \text{ K}, \text{ and } = 2 \text{ ms}$ 



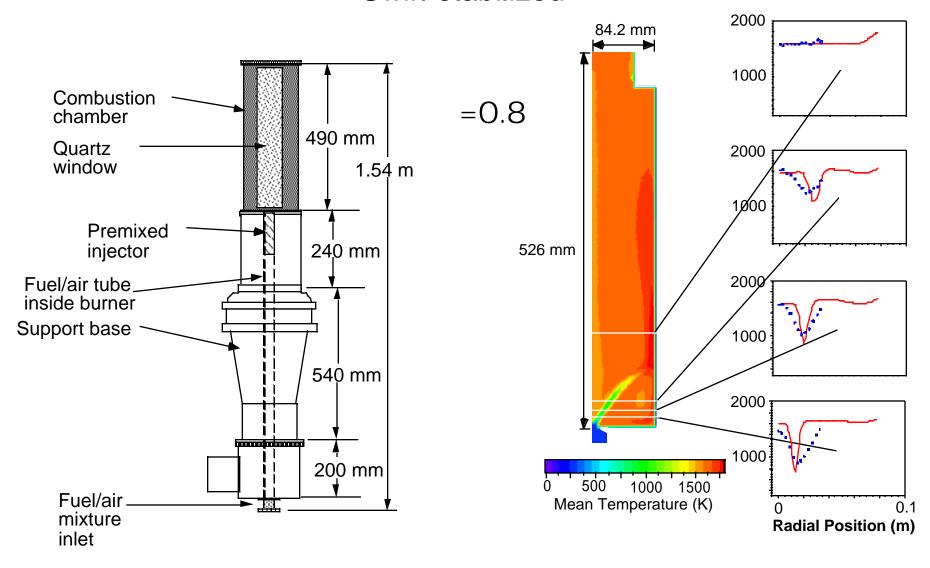
### **5-Step Chemistry**

Mallampalli et al., 1996

$$3H_2 + O_2 + CO = 3H_2O + CO$$
 $H_2 + 2OH = 2H_2O$ 
 $3H_2 + CO = H_2O + CH_4$ 
 $H_2 + CO_2 = H_2O + CO$ 
 $3H_2 + CO_2 = H_2O + CO$ 
 $3H_2 + CO + 2NO = 3H_2O + CO + N_2$ 

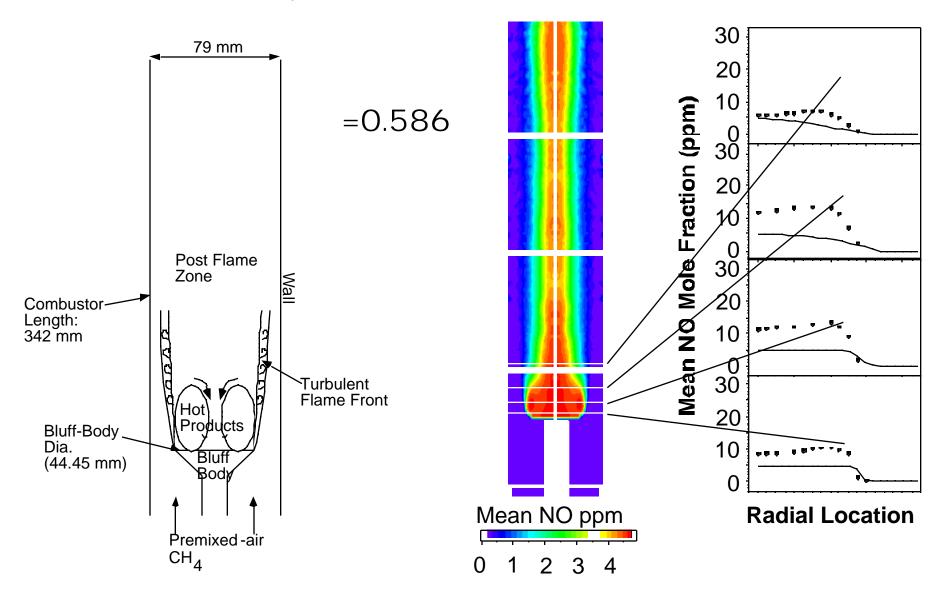
### **BYU Combustor**

#### Swirl-stabilized

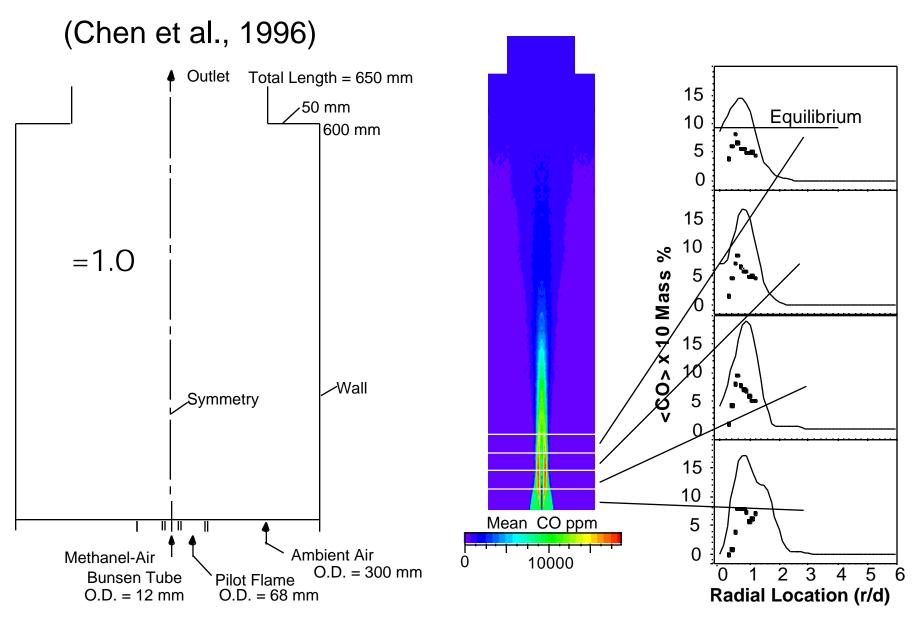


### **Vanderbilt Combustor**

Bluff-body stabilized (Nandula et al., 1996)

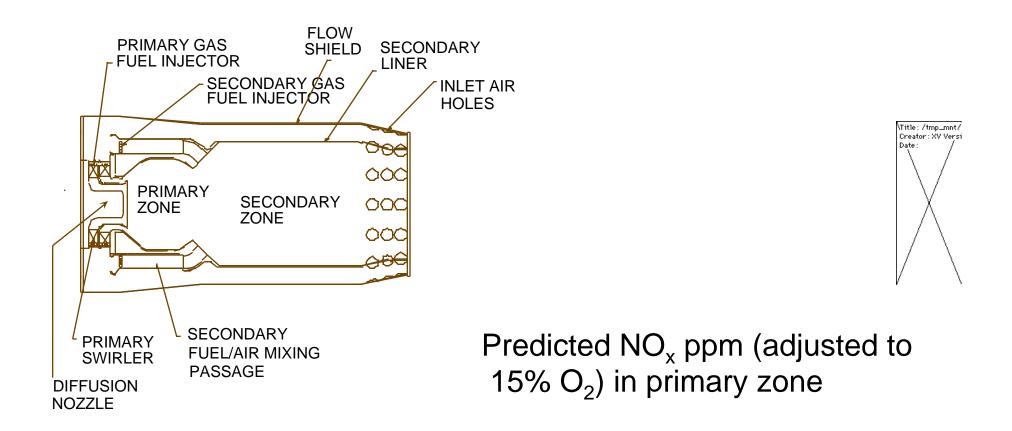


### **Piloted Bunsen Burner**



## **Westinghouse Combustor**

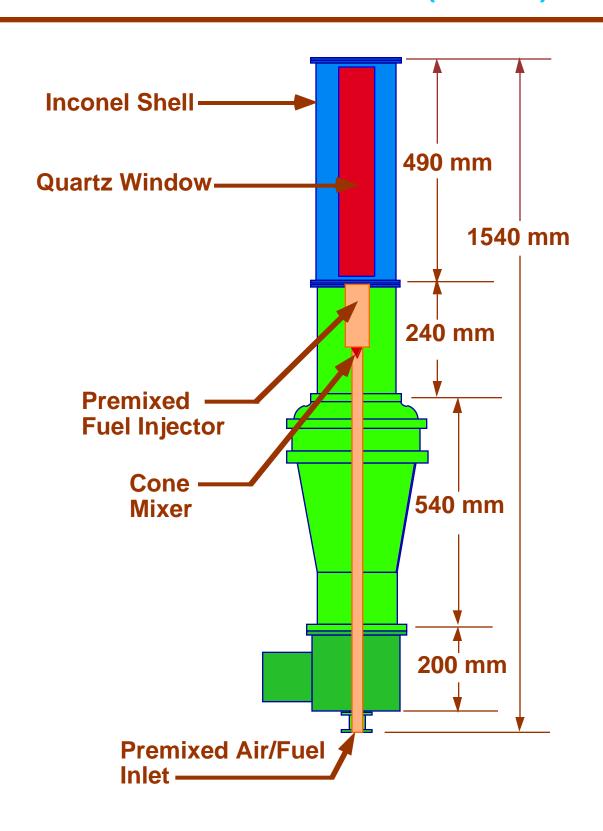
(Sharifi et al., 1995)



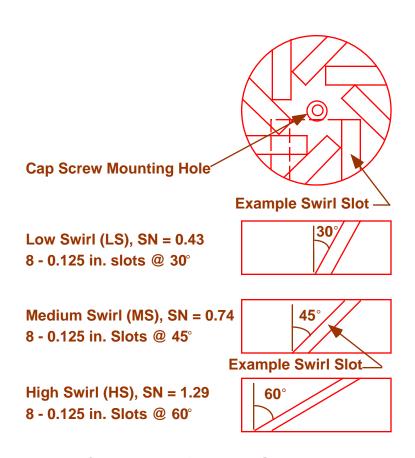
## **BYU Experimental Capability**

- Laboratory-scale, atmospheric pressure, model gas-turbine combustor (LSGTC) with good optical access
- Premixed and non-premixed fuel injectors
- Gaseous (nat'l gas and propane) and liquid (ethanol) fuels
- Optical instruments => instantaneous and non-intrusive
  - Film and video cameras => overall flame structure
  - CARS => T, CO, CO<sub>2</sub>, O<sub>2</sub> and N<sub>2</sub> directly H<sub>2</sub>O, and H<sup>\*</sup> and C<sup>\*</sup> by elemental balance
  - LDA => Axial, tangential or axial, radial velocities
  - PLIF => OH, CH, NO two-dimensional images

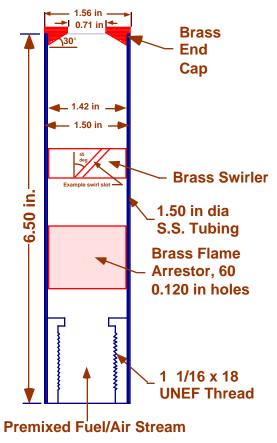
# **Atmospheric Laboratory-Scale Gas Turbine Combustor (LSGTC)**



#### **ATS Swirling, Turbulent, Premixed Fuel Injector**



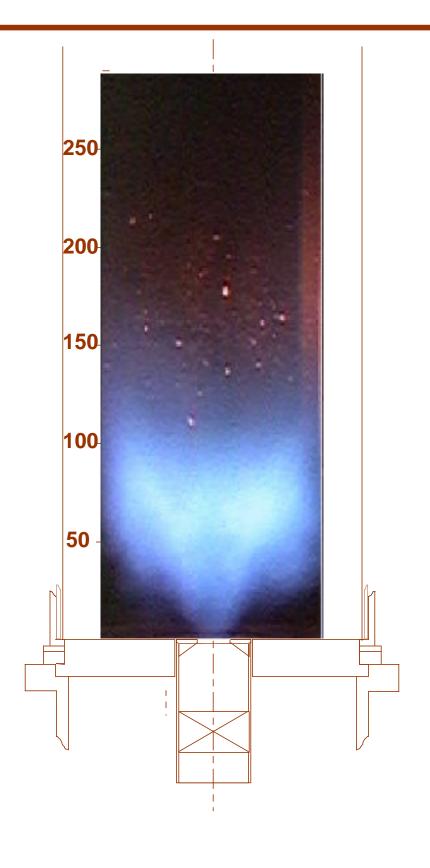
A) Details of Brass Swirlers



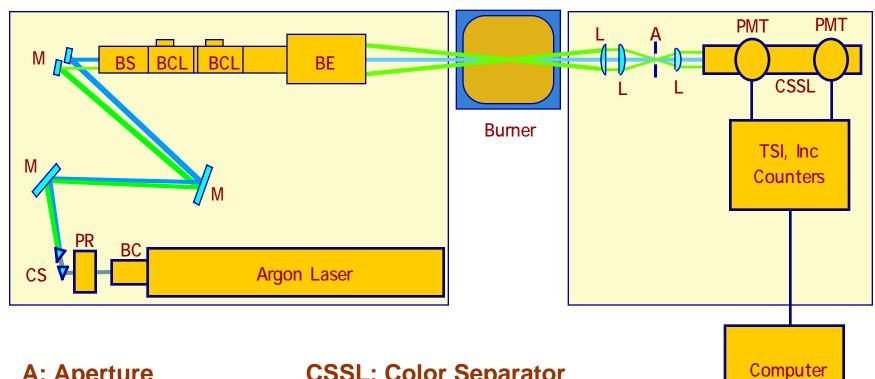
**B) ATS Premixed Burner Tube** 

#### **Video Image of Premixed Natural Gas/Air Flame**

(ATS-MS Burner, 500 slpm Air Flow Rate, = 1.0)



#### Schematic of LDA Installation on the LSGTC



A: Aperture

**BC: Beam Collimator** 

**BCL: Bragg Cell** 

**BE: Beam Expander** 

**BS: Beam Separator** 

**CS: Color Separator** 

**CSSL: Color Separator** 

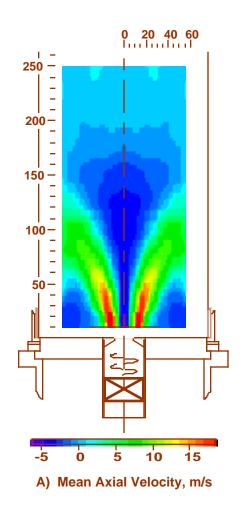
L: Lens

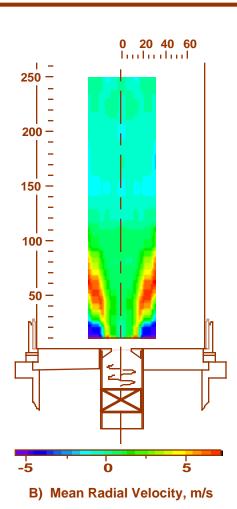
M: Mirror

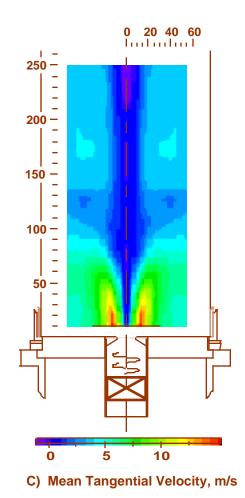
**PMT: Photomultiplier Tube** 

PR: Polarization Rotator

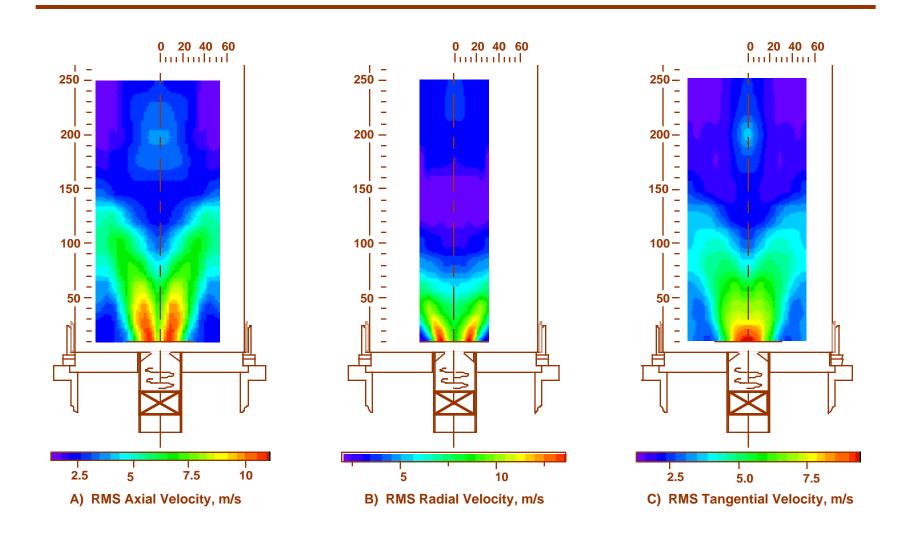
#### Iso-Velocity Contours in the LSGTC with the ATS-MS Burner



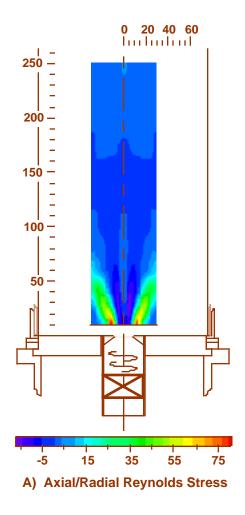


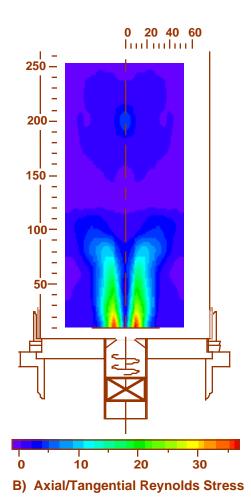


## RMS Velocity Contours in the LSGTC with the ATS-MS Burner (Premixed Natural Gas/Air, Air Flow Rate = 500 slpm, = 0.65)

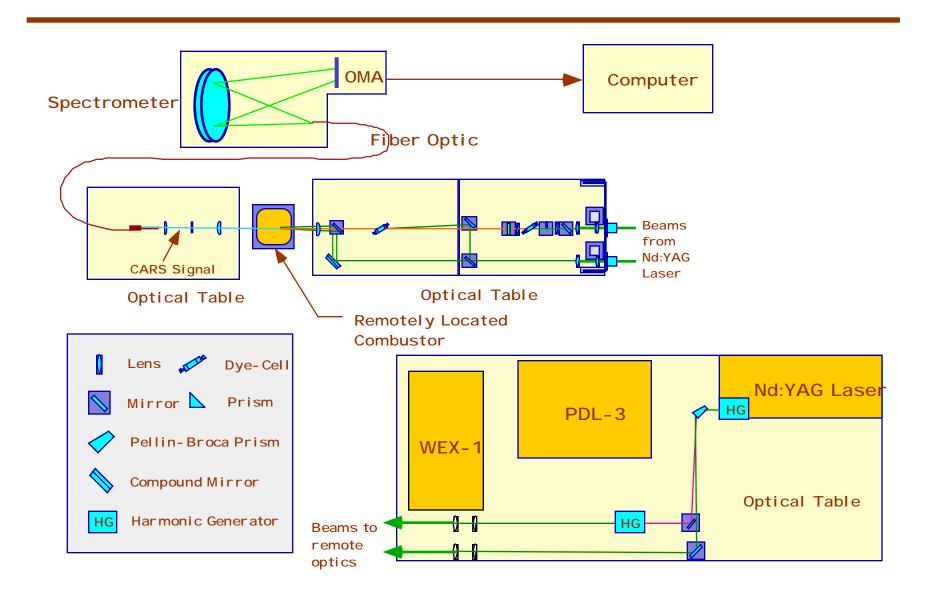


#### Reynolds Stress Contours in the LSGTC with the ATS-MS Burner

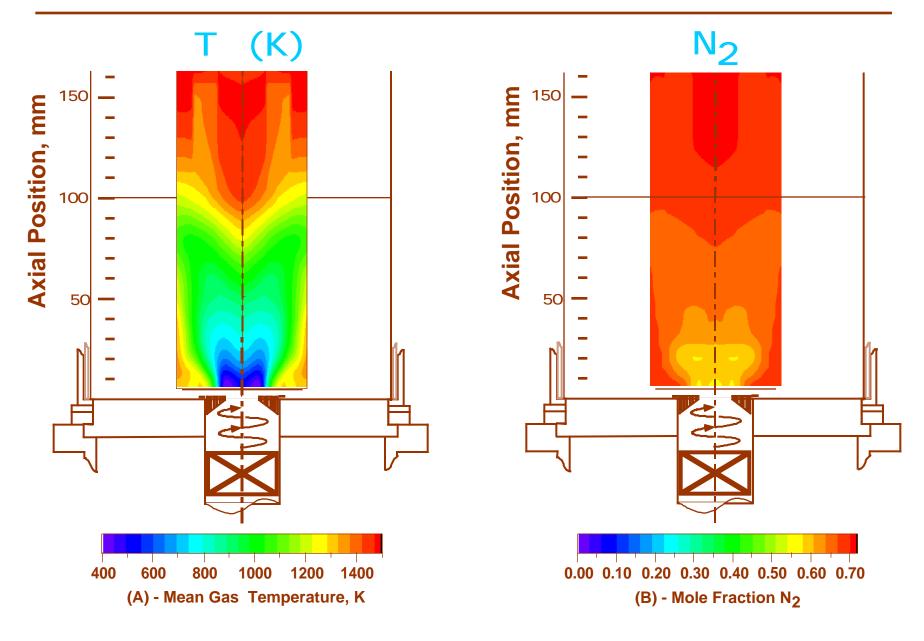




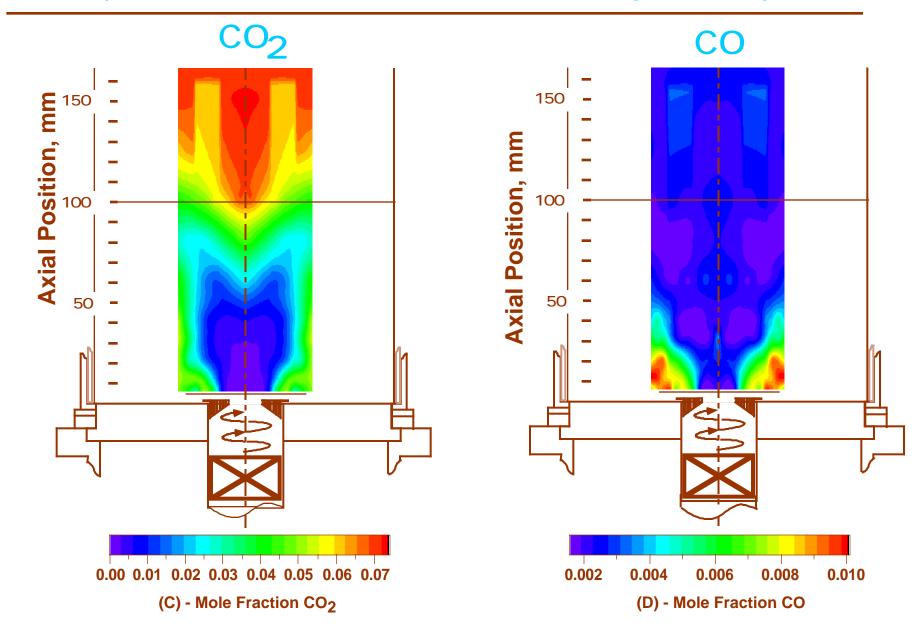
#### Schematic of Dual Dye, Single Stokes CARS Installation on the laboratory-Scale Gas Turbine Combustor (LSGTC)



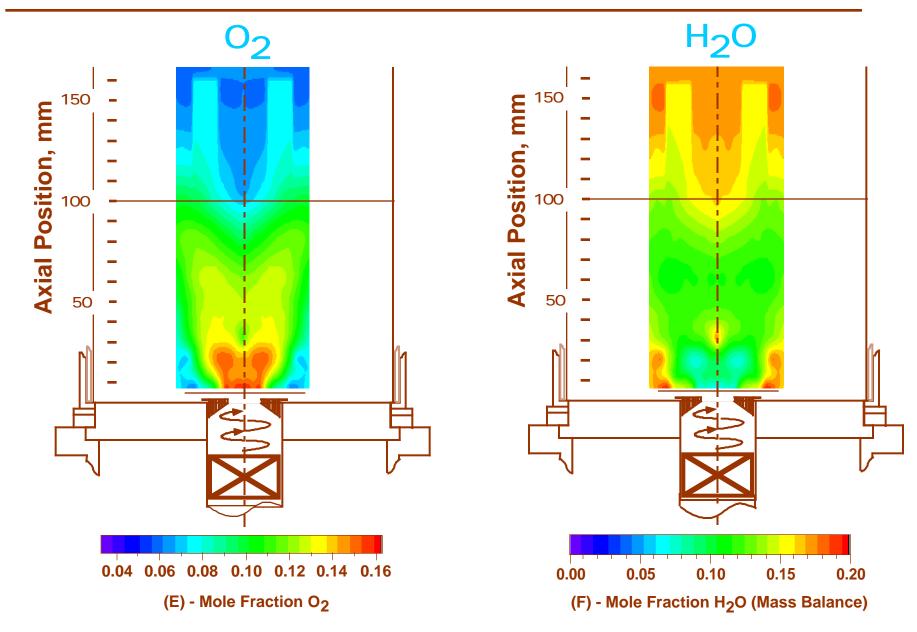
## Iso-Temperature and Iso-N<sub>2</sub> Concentration Contours with the ATS-MS Burner



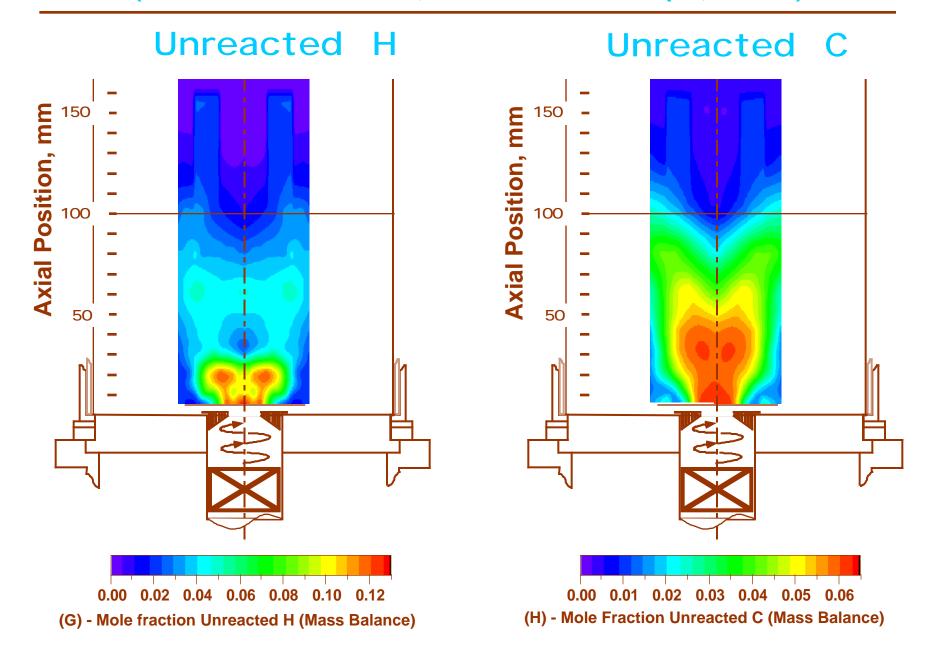
## Iso-CO<sub>2</sub> and Iso-CO Concentration Contours with the ATS-MS Burner



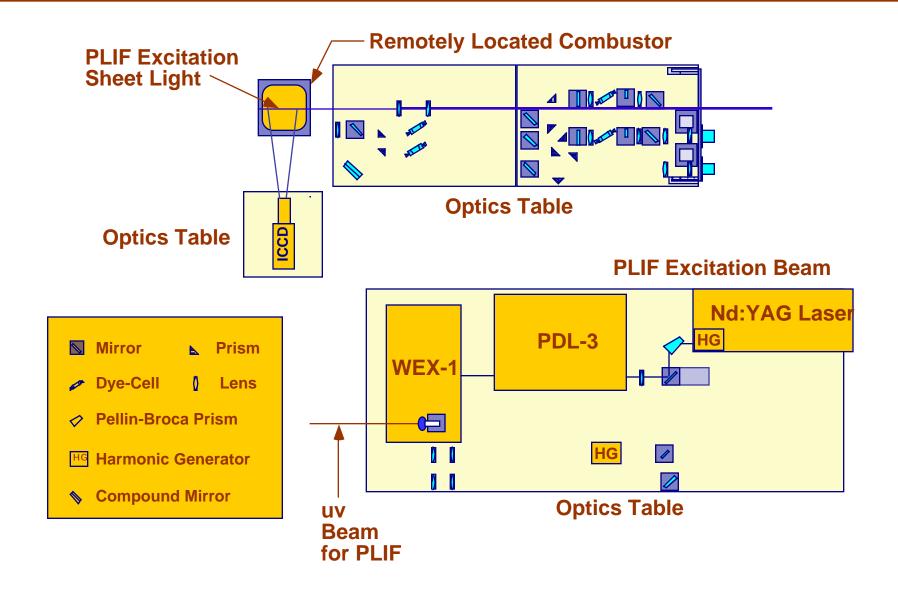
## Iso-O<sub>2</sub> and Iso-H<sub>2</sub>O Concentration Contours with the ATS-MS Burner



## Iso-Concentration Contours of Unreacted H and C with the ATS-MS Burner

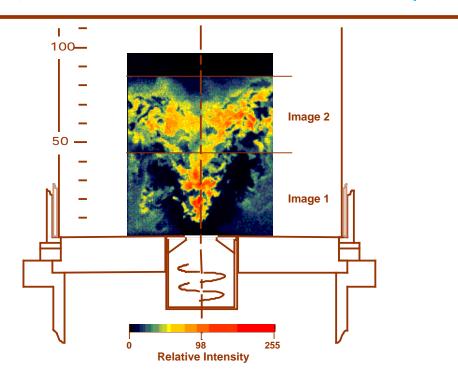


#### **Schematic of PLIF Installation on the LSGTC**



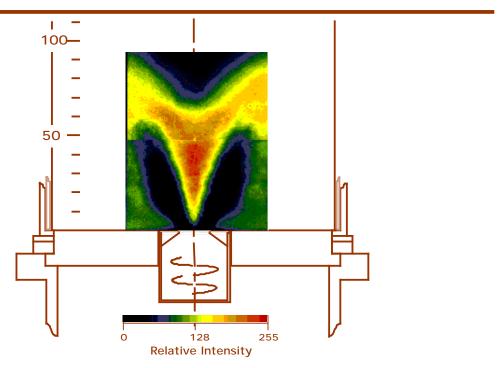
#### **Example Instantaneous PLIF Images of OH Radical**

(ATS-MS Burner, Premixed Natural Gas/Air, Air Flow Rate = 500 slpm, = 0.80)



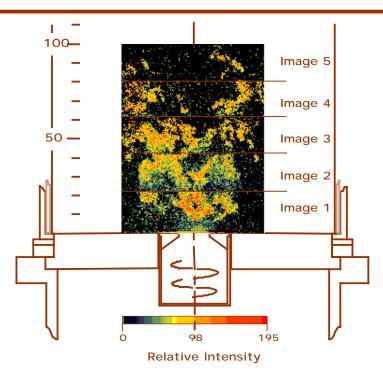
#### Mean of 128 Instantaneous PLIF Images of OH Radical

(ATS-MS Burner, Premixed Natural Gas/Air, Air Flow Rate = 500 slpm, = 0.80)



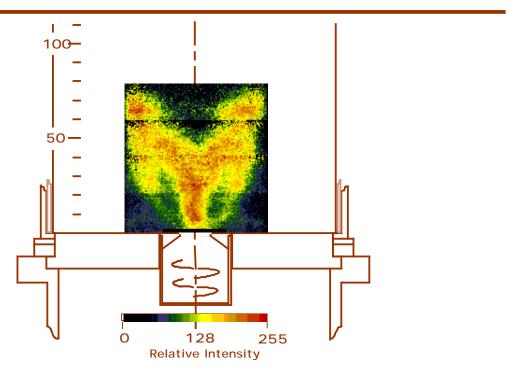
#### **Example Instantaneous PLIF Images of CH Radical**

(ATS-MS Burner, Premixed Natural Gas/Air, Air Flow Rate = 500 slpm, = 0.80)

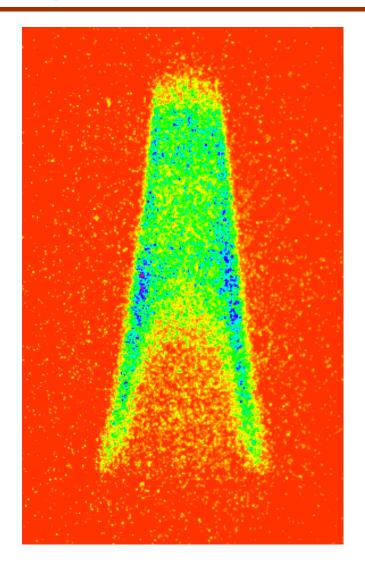


#### Mean of 64 Instantaneous PLIF Images of CH Radical

(ATS-MS Burner, Premixed Natural Gas/Air, Air Flow Rate = 500 slpm, = 0.80)



## NO PLIF Image in a Laminar, Premixed Ethylene/Air Flame (ca 225.6 nm Pump Laser; ca 234-237 nm Fluorescence)



### **Conclusions/Results**

- New model for lean premixed systems
- New reduced mechanisms for lean premixed combustion
- Temperature, species, and PLIF image data obtained in laboratory-scale gas turbine combustor
- Reasonable comparisons with data from laboratory combustors
- First ever predictions of NO in premixed methane flame with PDF method
- First practical 3-D combustion calculations with velocityscalar PDF method
- Code user's manual written
- Code available for beta testing

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- BEAM Tech., Inc., Dr. Gal Berkooz and Prof. Pope for use of PDF2DS, a 2-dimensional PDF program
- Prof. Robert Pitz and students at Vanderbilt U. for lean premixed flame data
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